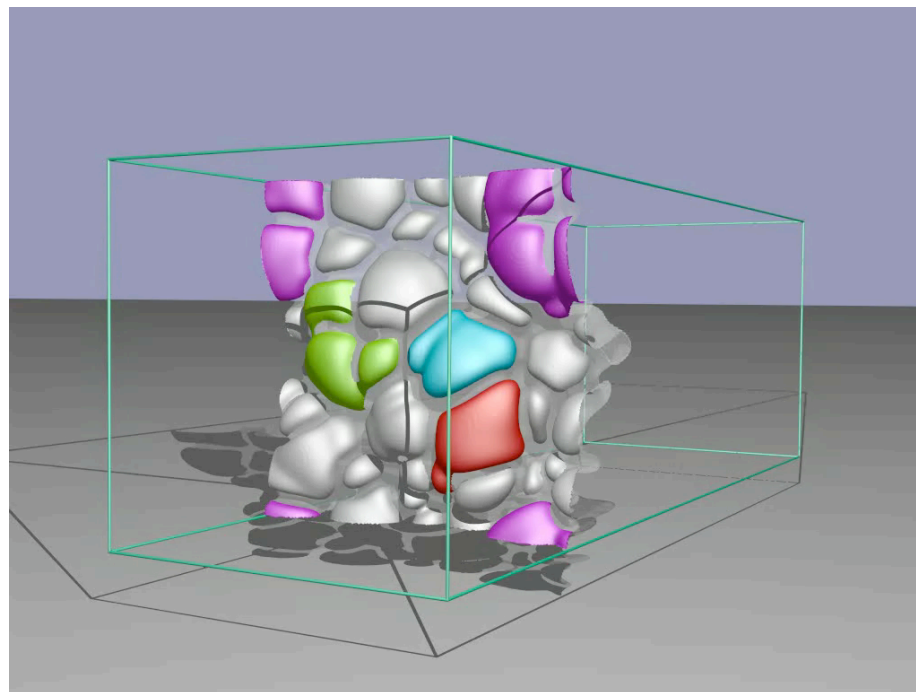


VACET



Multi-scale Morse Analysis of Scientific Data: Understanding Turbulence in Hydrogen Flames



Valerio Pascucci

Scientific Computing and Imaging Institute
School of Computing,
University of Utah



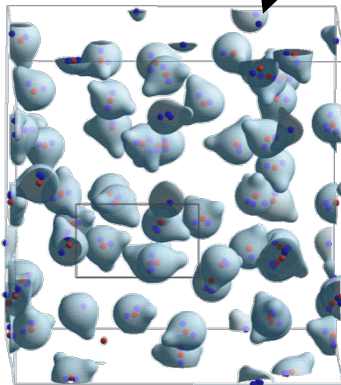
Massive Scientific Simulations are Source of Great Challenges and Opportunities



BlueGene/L



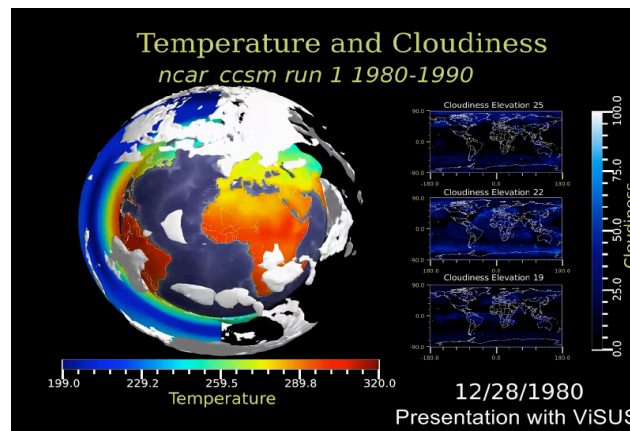
Roadrunner



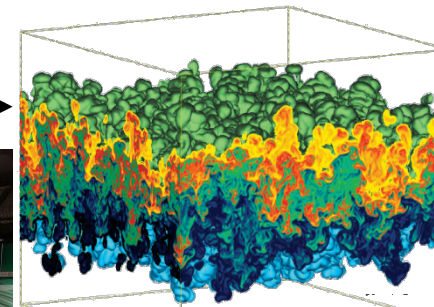
Molecular Dynamics



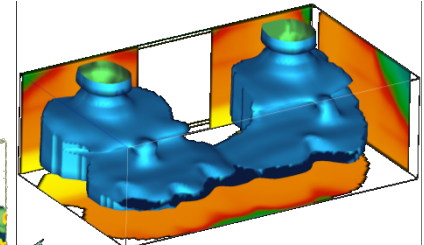
Jaguar



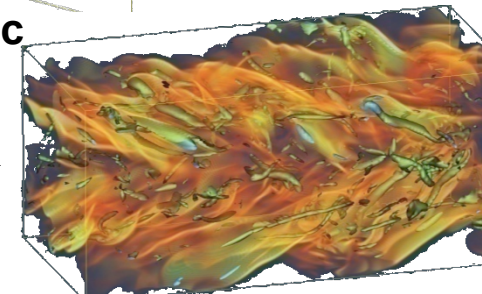
Climate Modeling



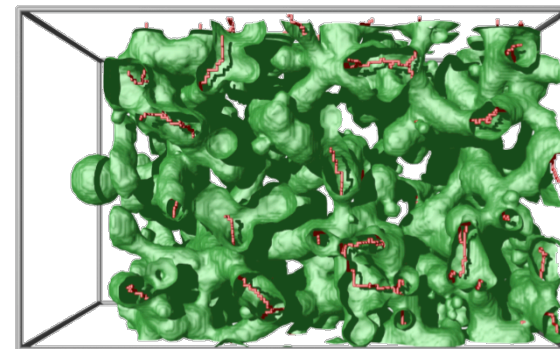
Hydrodynamic Instabilities



Subsurface Modeling



Combustion Simulations

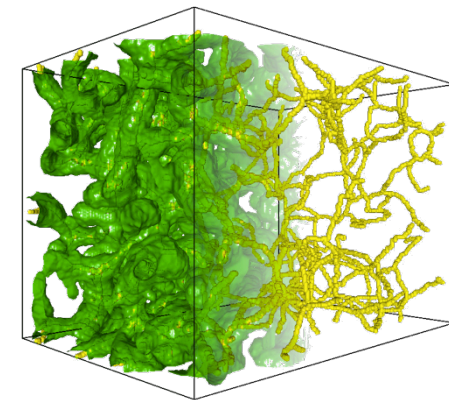
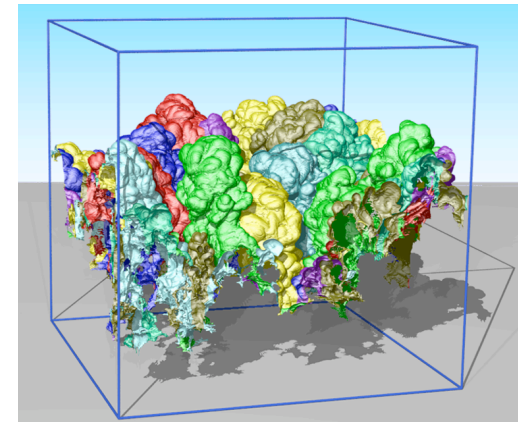


Material Sciences

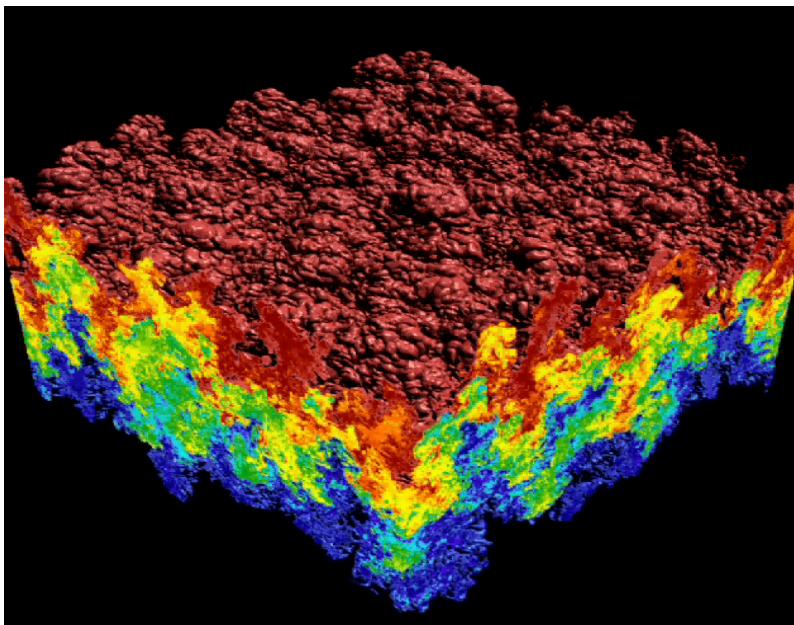
Traditional Data Analysis Tools are Often Ineffective for Petascale Models



- **Massive scientific models are challenging due to:**
 - Sheer volume of information
 - Complexity of the information
- **Tools do not scale with the data sizes**
- **Difficult to capture multiple scales**
- **Numerical methods unstable and sensitive to noise**
- **Difficulty in providing error bounds associated with the coarse scale analysis**
- **Lack of a mathematical language: hard to reproduce results and map them to new definitions**

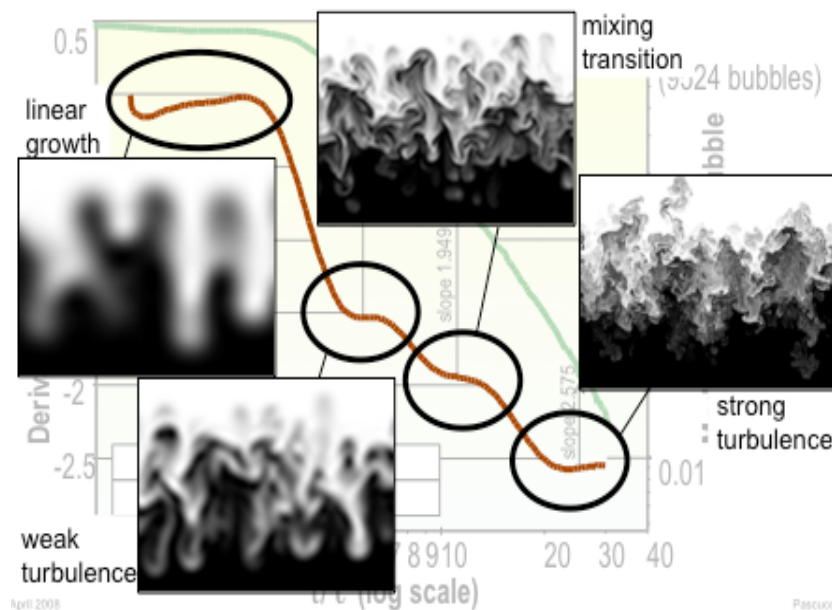
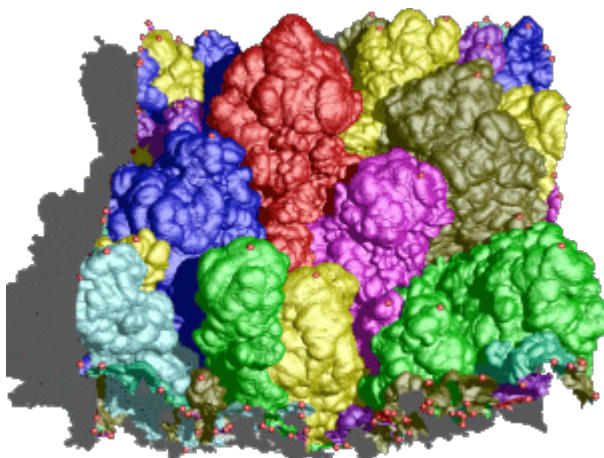


We Focus on Quantitative Analysis for Answering Science Questions

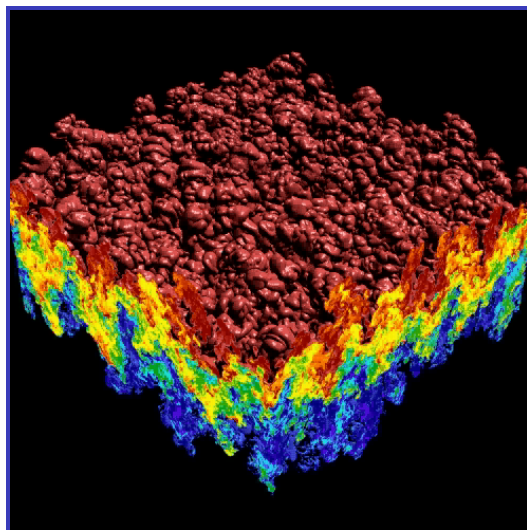
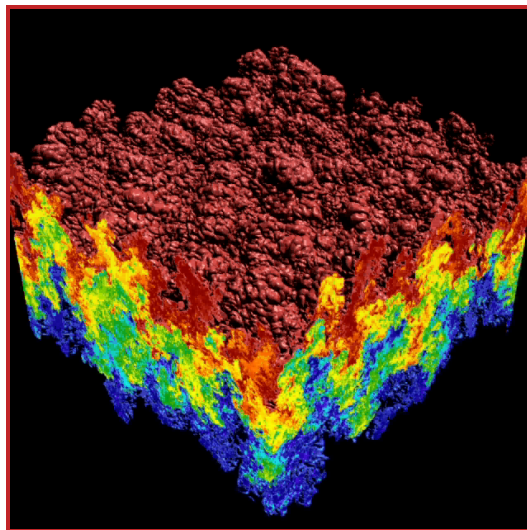


Rayleigh–Taylor Instability (fusion, super-novae, ...).

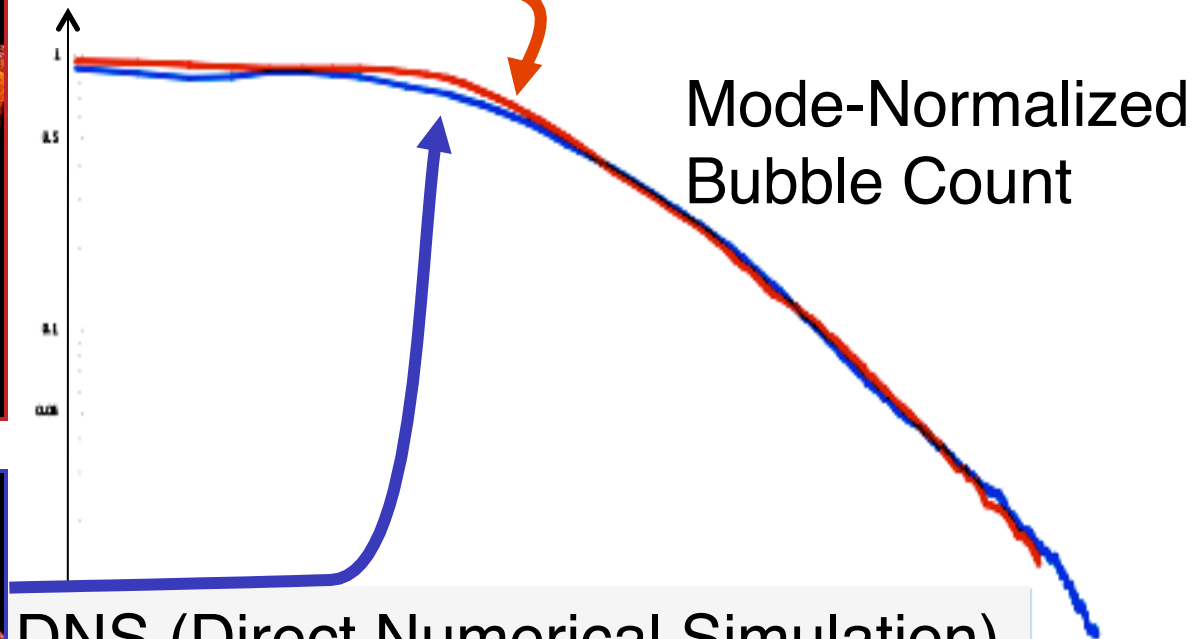
- What are the stages of the turbulent mixing process?
- Over 40 TB



We Provided the First Feature-Based Validation of a LES with Respect to a DNS



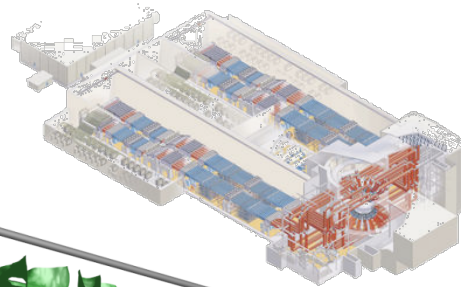
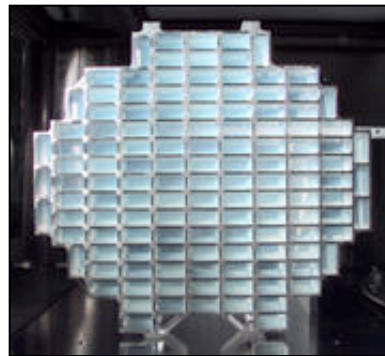
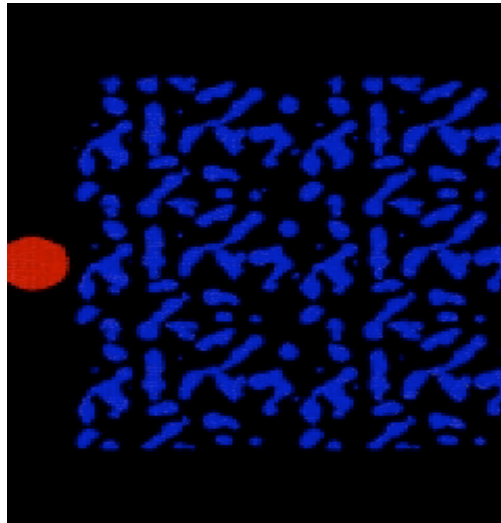
LES (Large Eddy Simulation) 25TB



DNS (Direct Numerical Simulation)
40 TB

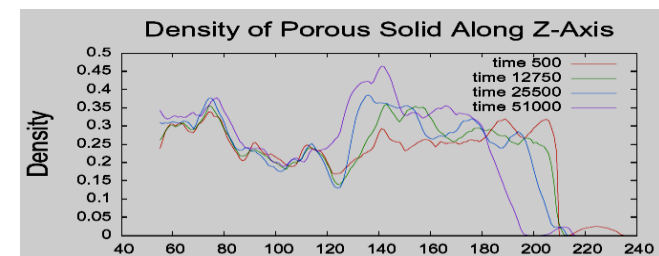
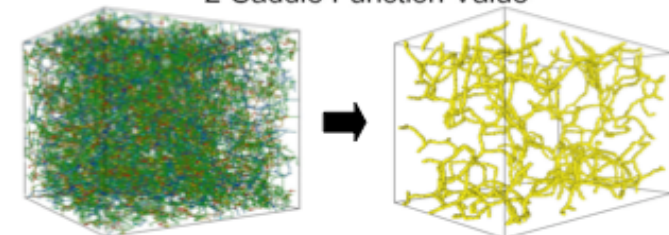
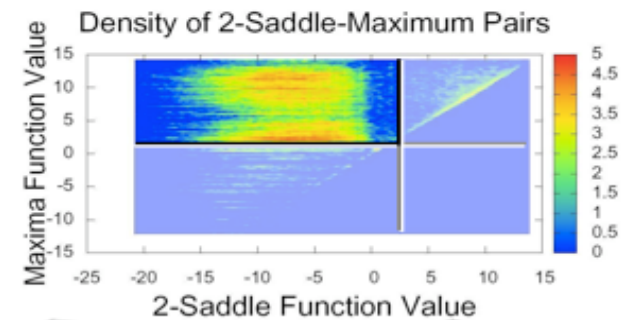
Normalized Time

Quantitative Analysis of the Impact of a Micrometeoroid in a Porous Medium



Many possible applications:

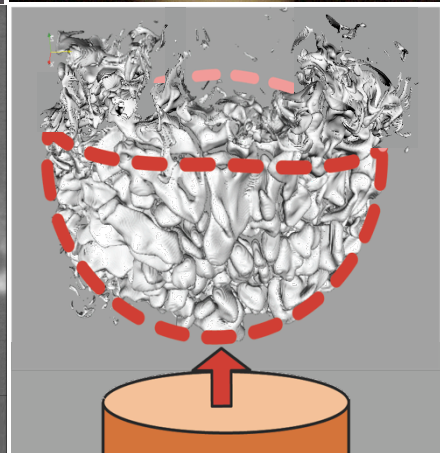
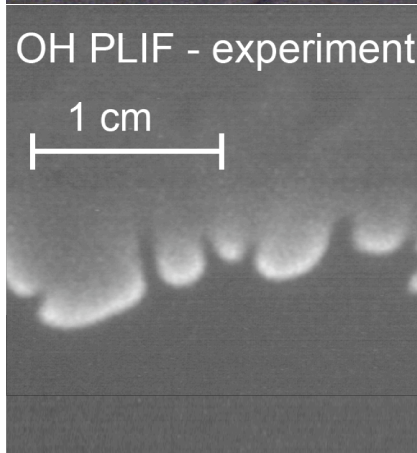
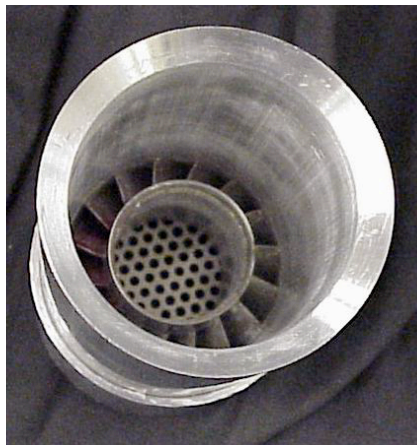
- NASA's Stardust Spacecraft
- National Ignition Facility Targets
- Light and Robust Materials
- 8 TB each variable



Pascucci-6



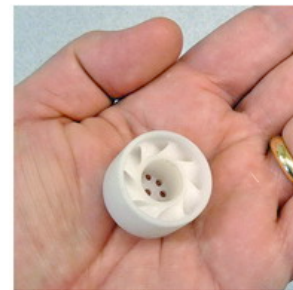
Understanding Turbulence for Low Emission, High Efficiency Combustion



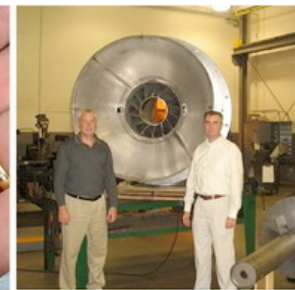
Experiment

Simulation

- Lean premixed H_2 flames
- Low Swirl Combustion (LSC) Burners
- Low pollution in energy production
- High Efficiency in fuel consumption
- Scalable from residential to industrial use
- Each variable 3.9-4.5 TB

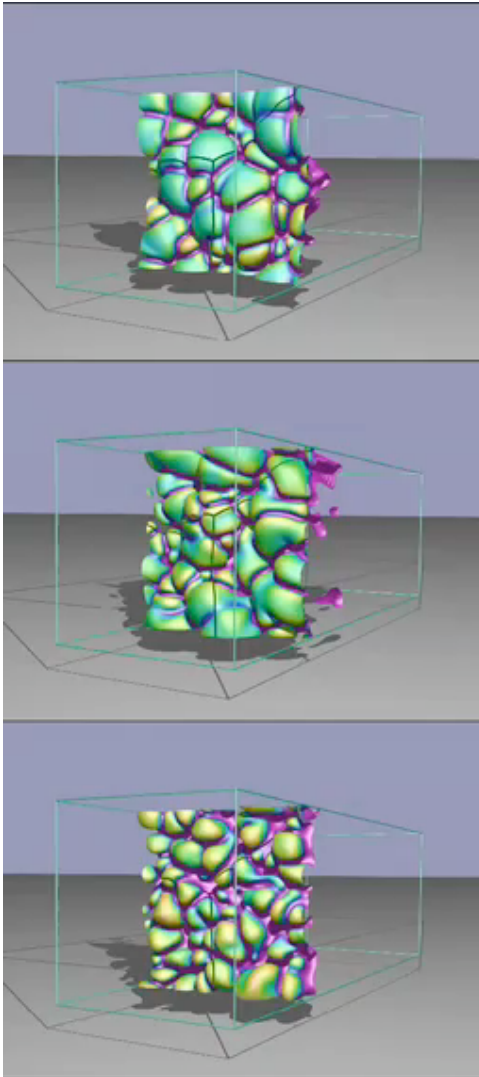


1" burner (5 kW, 17 KBtu/hr)



28" burner (44 MW, 150 MBtu/hr)

We Take on the Challenge of Developing a Quantitative Analysis Detecting Turbulence



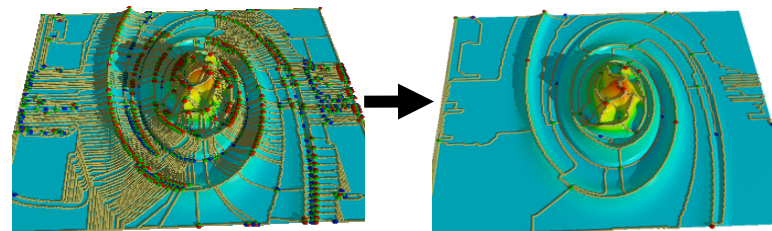
Understanding combustion processes over a broad range of burning conditions is an important problem for designing engines and power plants.

- **Simulation with AMR mesh.**
- **Simulations of lean premixed hydrogen flames with three degrees of turbulence.**
- **Can we identify precisely and track in time burning regions?**
- **Can we discriminate the degree of turbulence from a quantitative analysis?**

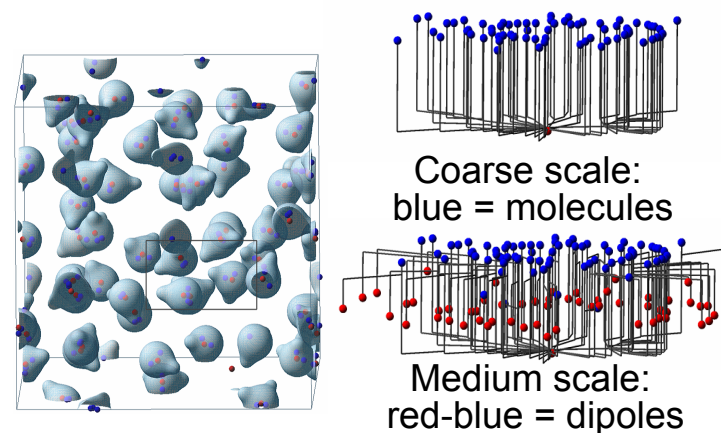
We Introduced Robust Topological Methods for Quantitative Data Analysis



- Provably robust computation
- Provably complete feature extraction and quantification
- Hierarchical topological structures used to capture multiple scales
- Error-bounded approximations associated with each scale
- Formal mathematical definition associated with each analysis
- Scalable performance in association with streaming techniques



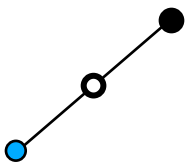
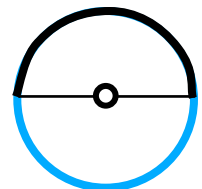
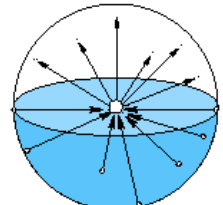
Hierarchical topology of a 2D Miranda vorticity field



Molecular dynamics simulation (left) with abstract graph representation of its features at two scales (right)

We Rewrote Morse Theory for Provably Robust and Correct Computations



	$f(x) : D \rightarrow \mathbb{R}$	$F(x) : S \rightarrow \mathbb{R}$
	Classical mathematical definitions	Simulation of differentiability
domain	D smooth manifold	S simplicial complex
function	f infinitely differentiable	$F(x)$ PL-extension of $f(x_i)$
critical point	$\nabla f(p) = 0$ numerical  1D	$LowerLink(p) \neq B^{d-1}$ combinatorial  2D
		 3D

Independent local computation yield globally consistent results

We Introduced New Techniques for Critical Point Classification



type	index
Minimum	0
\vdots	\vdots
Saddle	$d-1$
Maximum	d

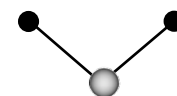
$$\nabla f(p) = 0$$

$$f(x)|_p = f(p) + \sum_{i=1}^{d-k} x_i^2 - \sum_{j=d-k+1}^d x_j^2$$

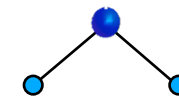
numerical

The Morse Lemma

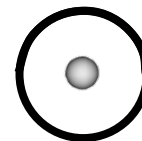
There are $d+1$ types
of critical points



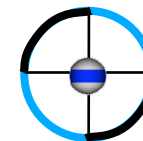
Minimum



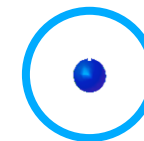
Maximum



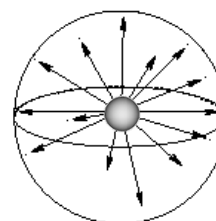
Minimum



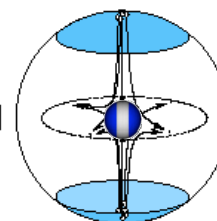
Saddle



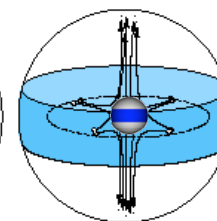
Maximum



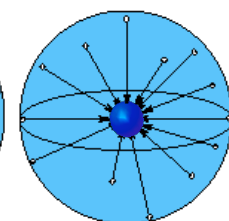
Minimum



1-saddle



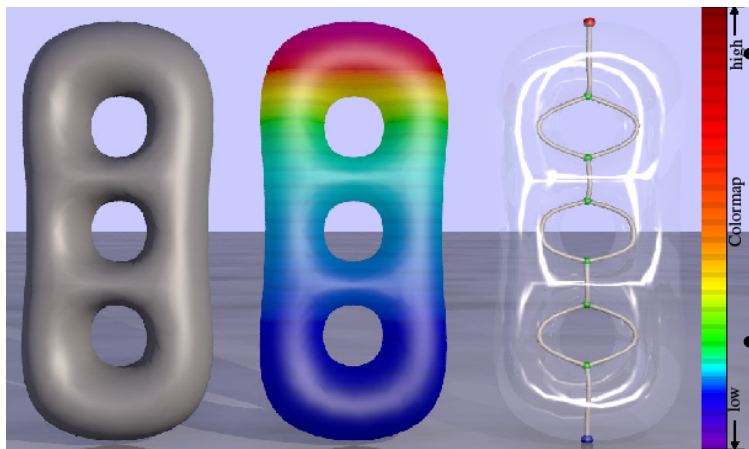
2-saddle



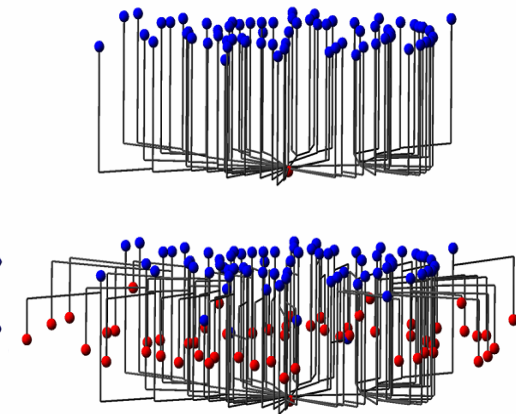
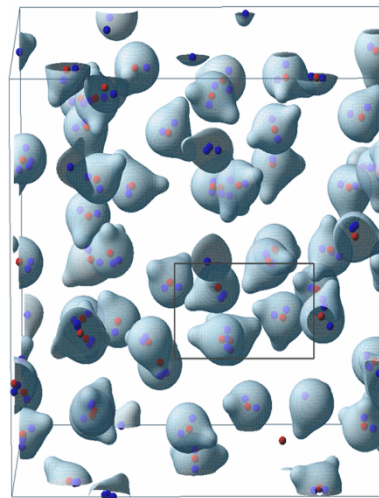
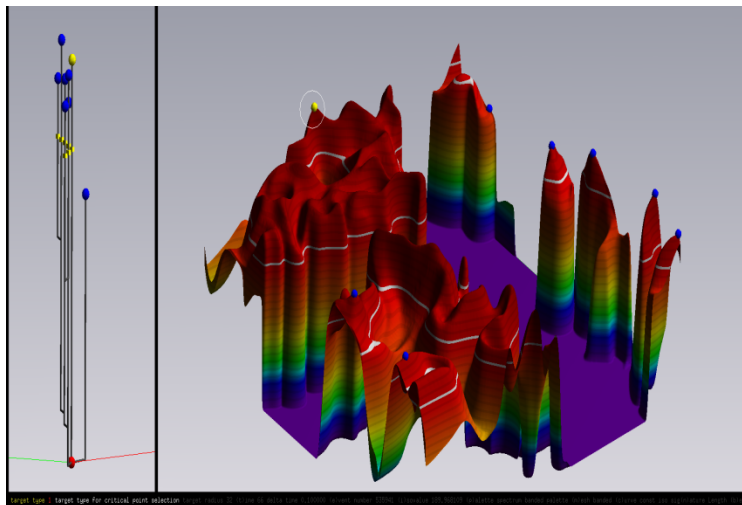
Maximum

combinatorial

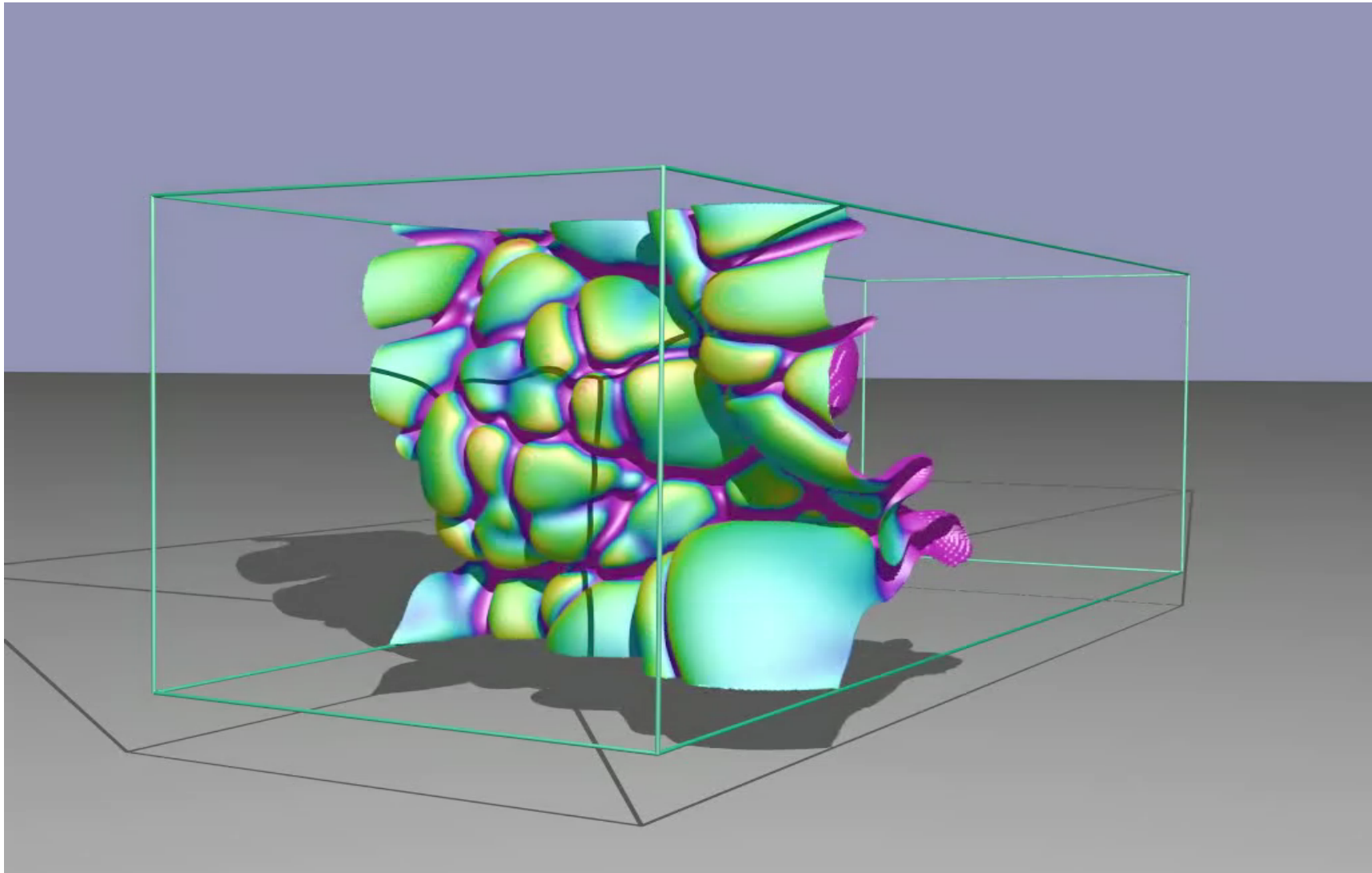
Topological Constructs Allow Building Effective and Succinct Shape Descriptors



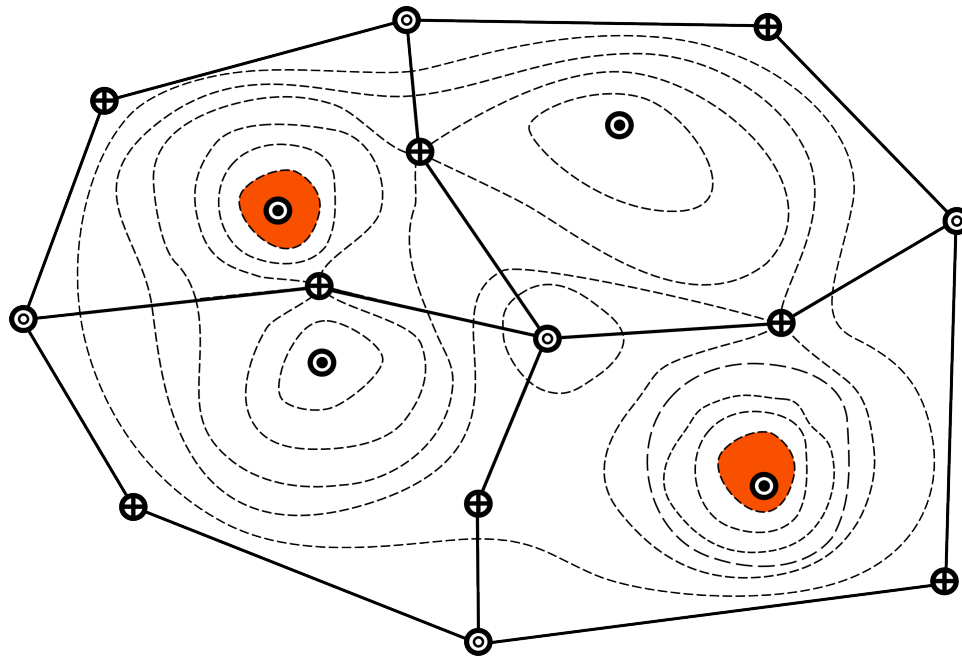
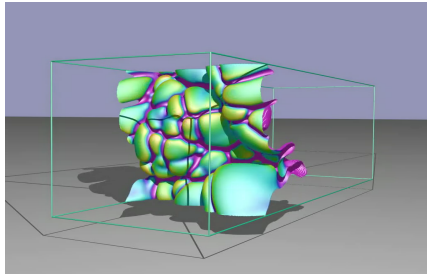
- The **Reeb graph** is the graph obtained by continuous contraction of all the contours in a scalar field, where each contour is collapsed to a distinct point.
- First algorithms for **robust** and **accurate** computation of Reeb graphs in any dimension.



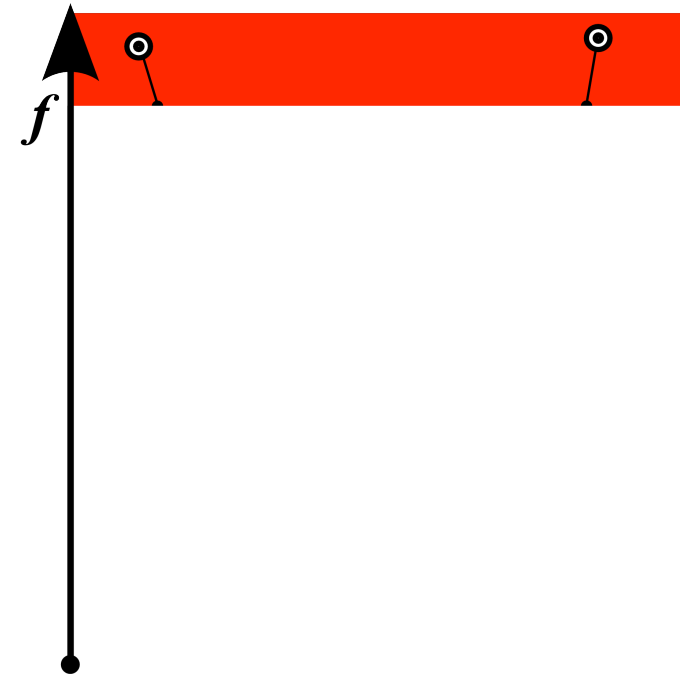
We build a hierarchical Morse complex of H2 consumption on an isothermal surface



We build a hierarchical Morse complex of H2 consumption on an isothermal surface

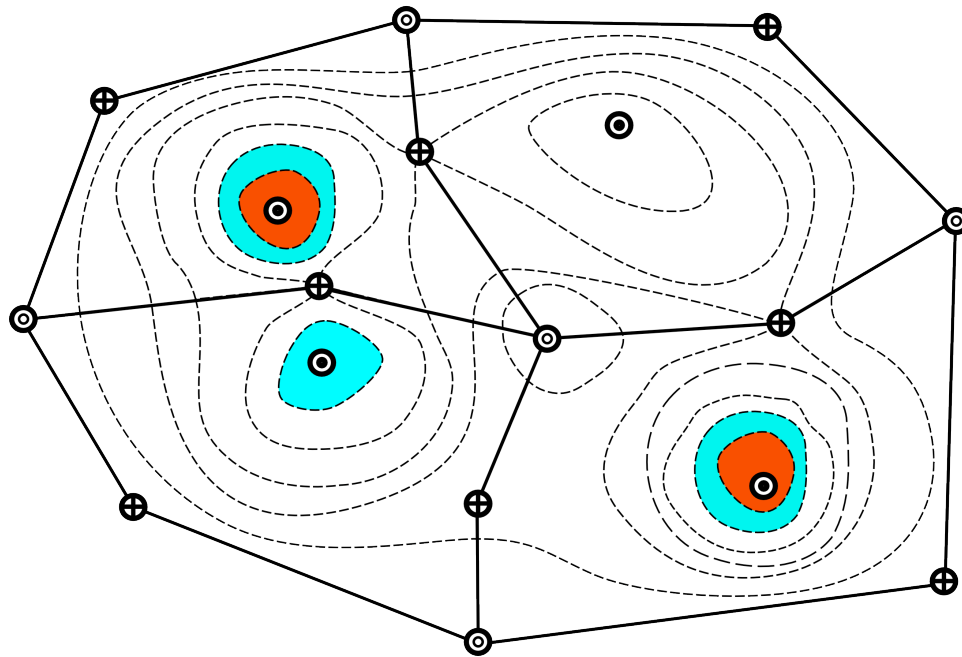
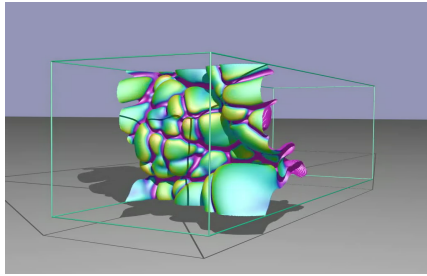


domain

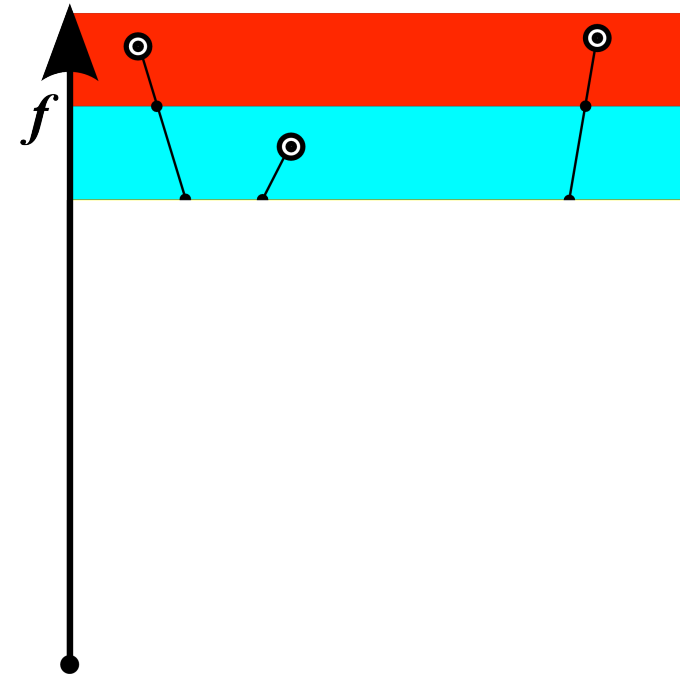


hierarchy

We build a hierarchical Morse complex of H2 consumption on an isothermal surface

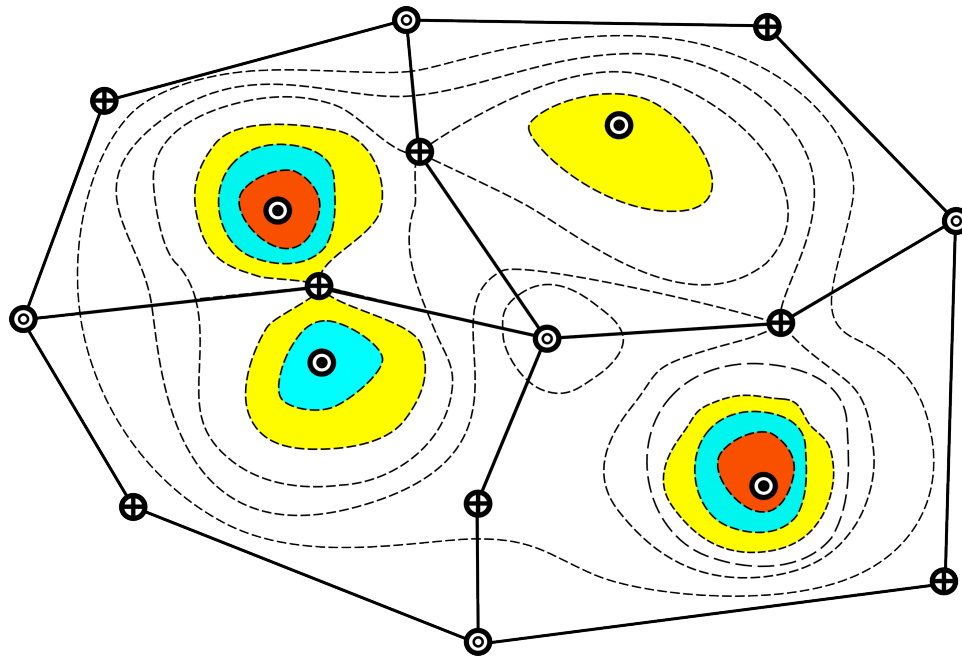
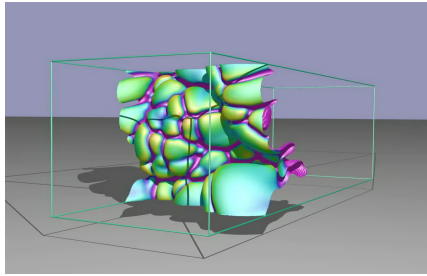


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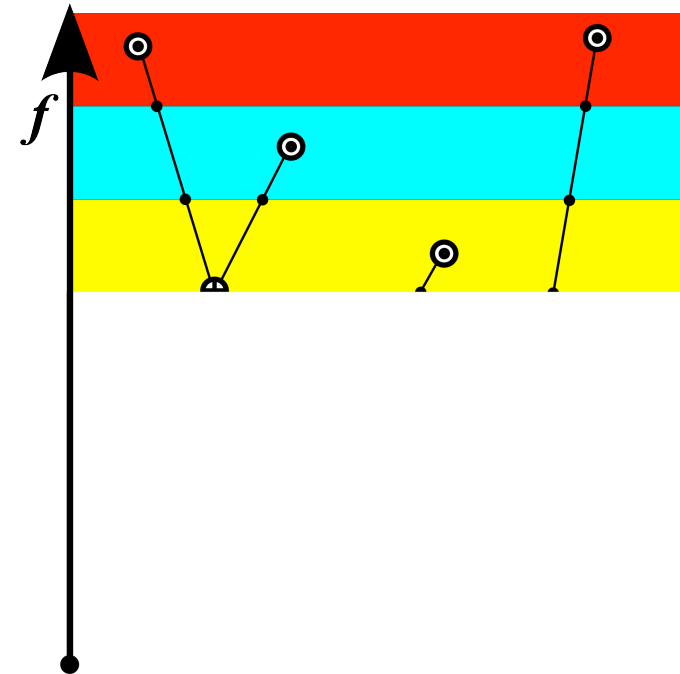


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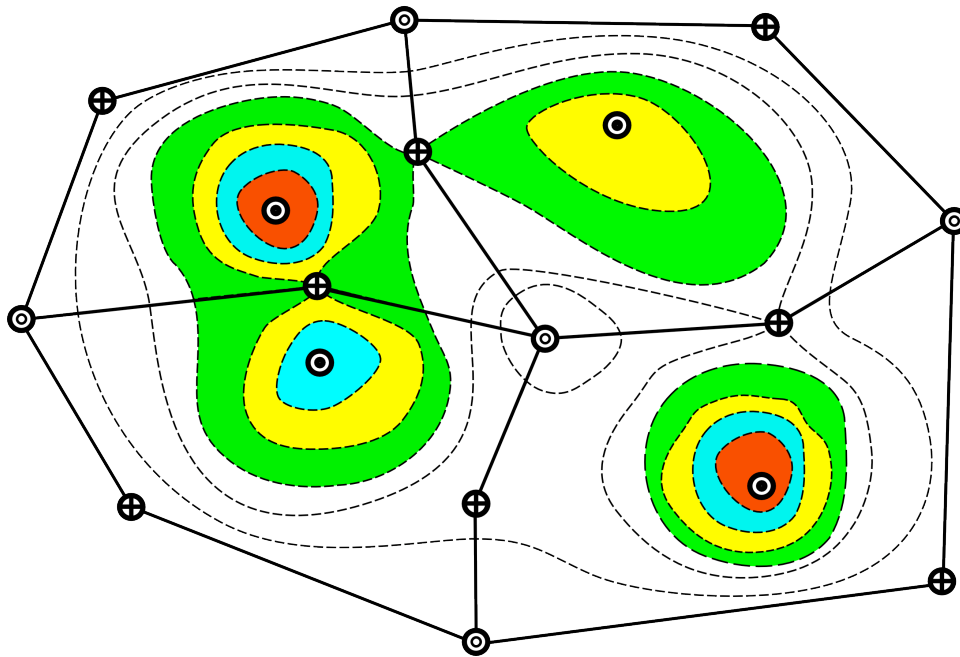
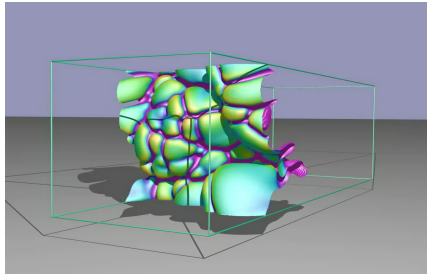


domain

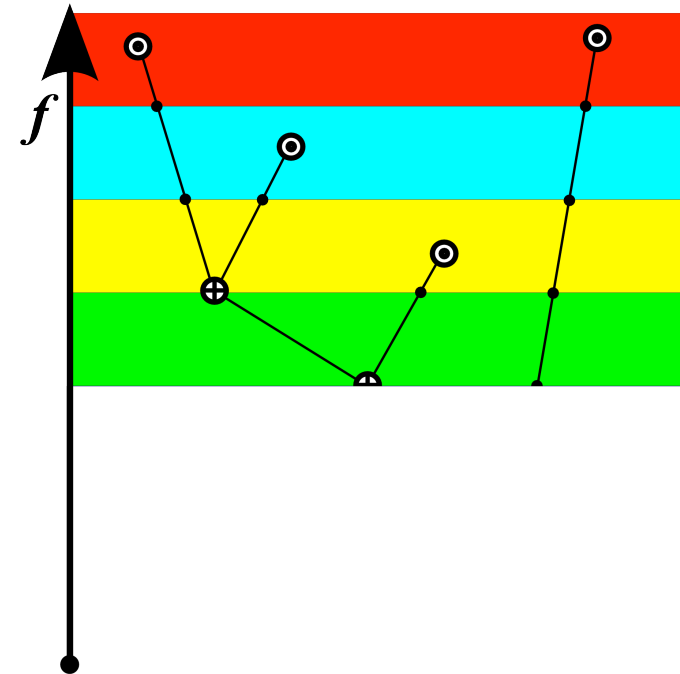


hierarchy

We build a hierarchical Morse complex of H2 consumption on an isothermal surface

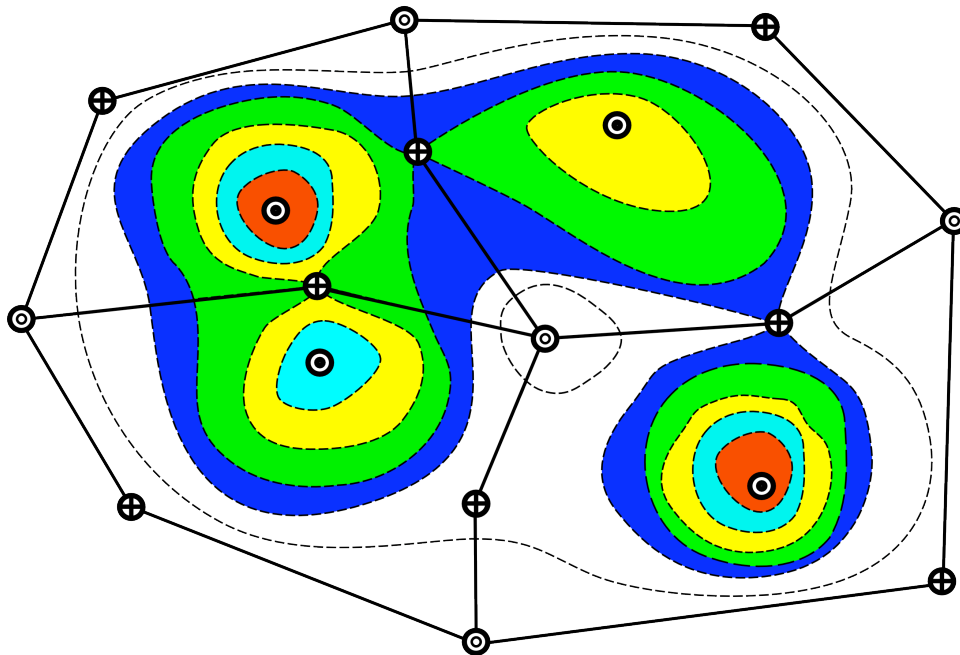
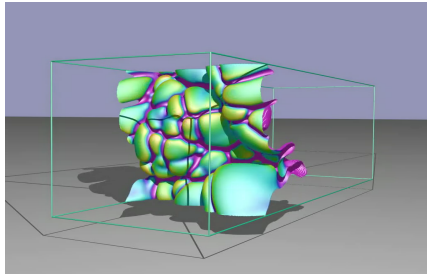


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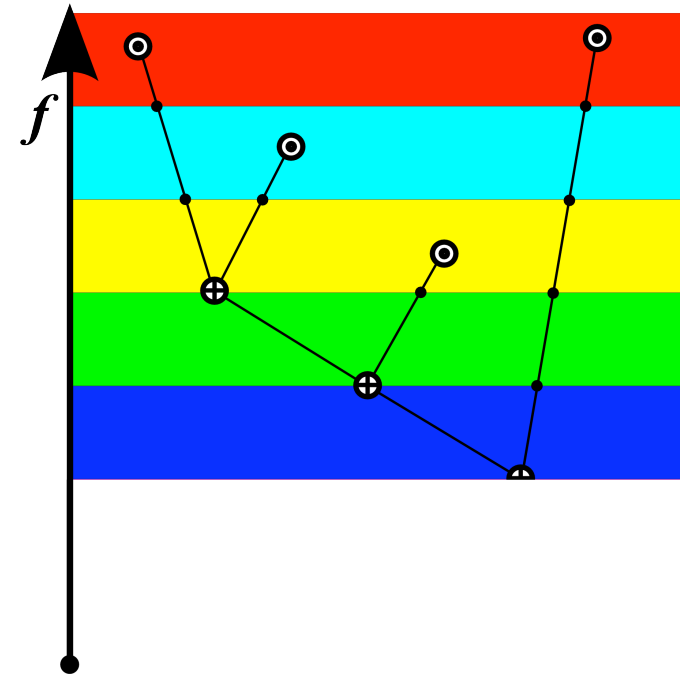


hierarchy

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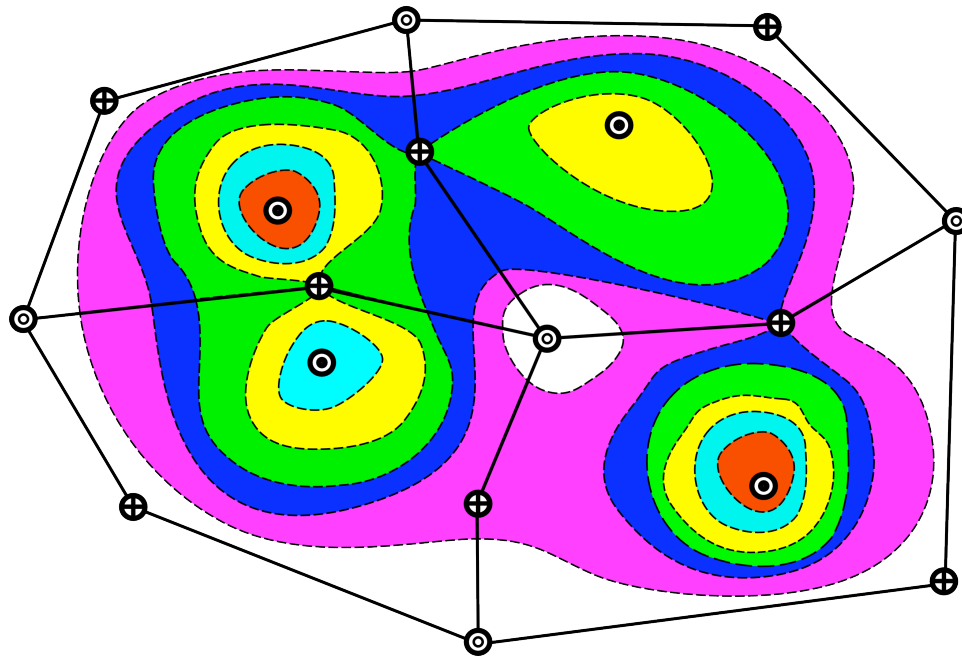
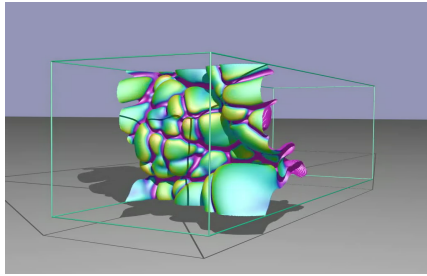


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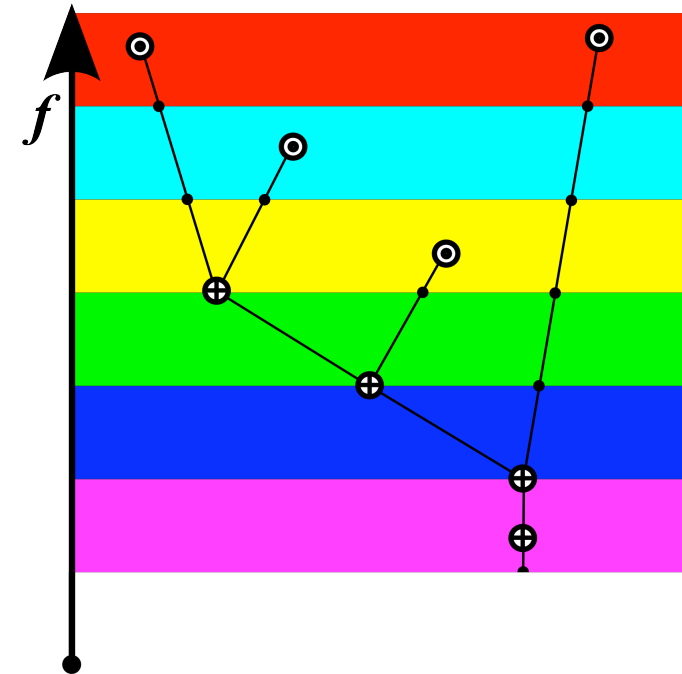


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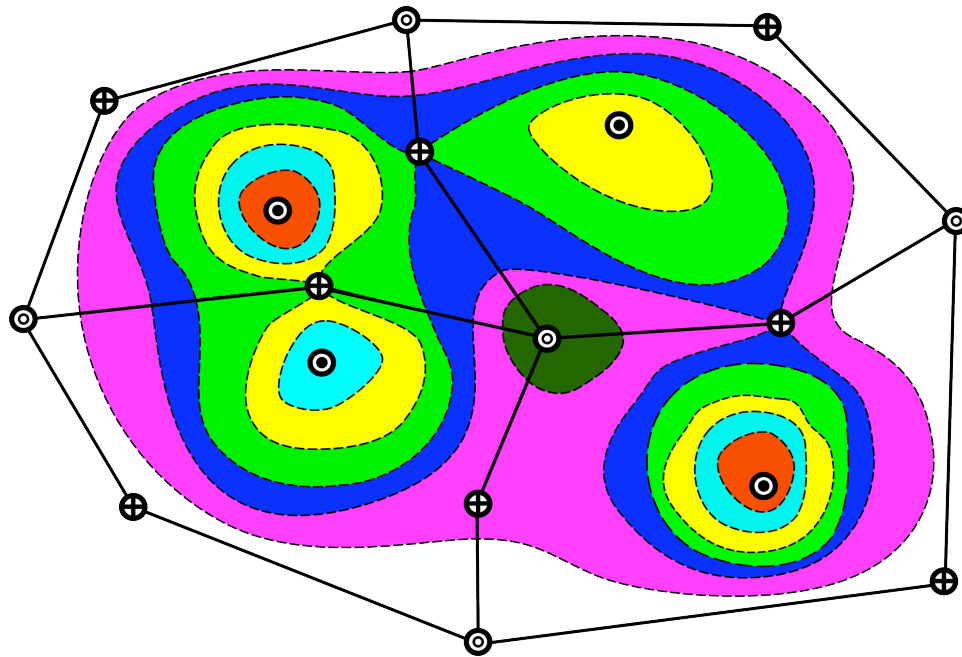
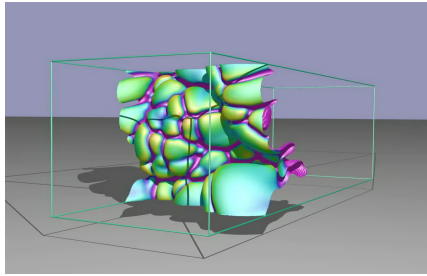


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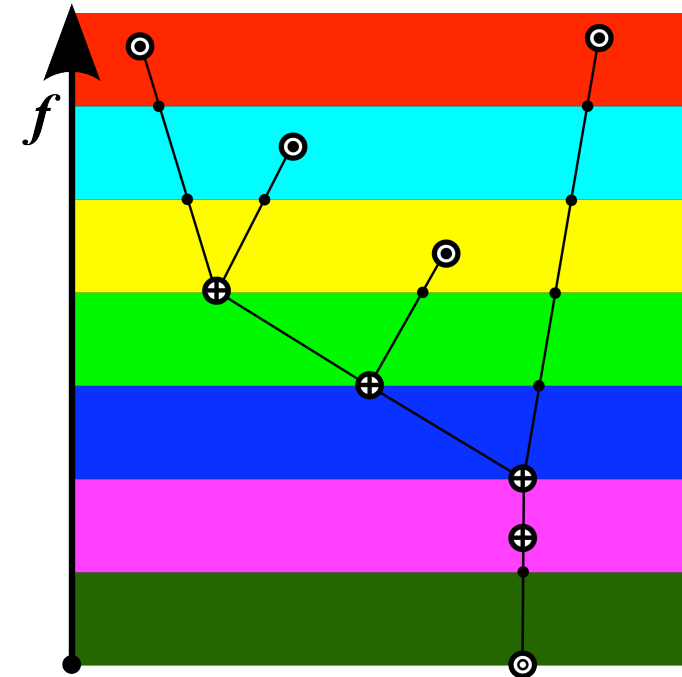


hierarchy

We build a hierarchical Morse complex of H2 consumption on an isothermal surface

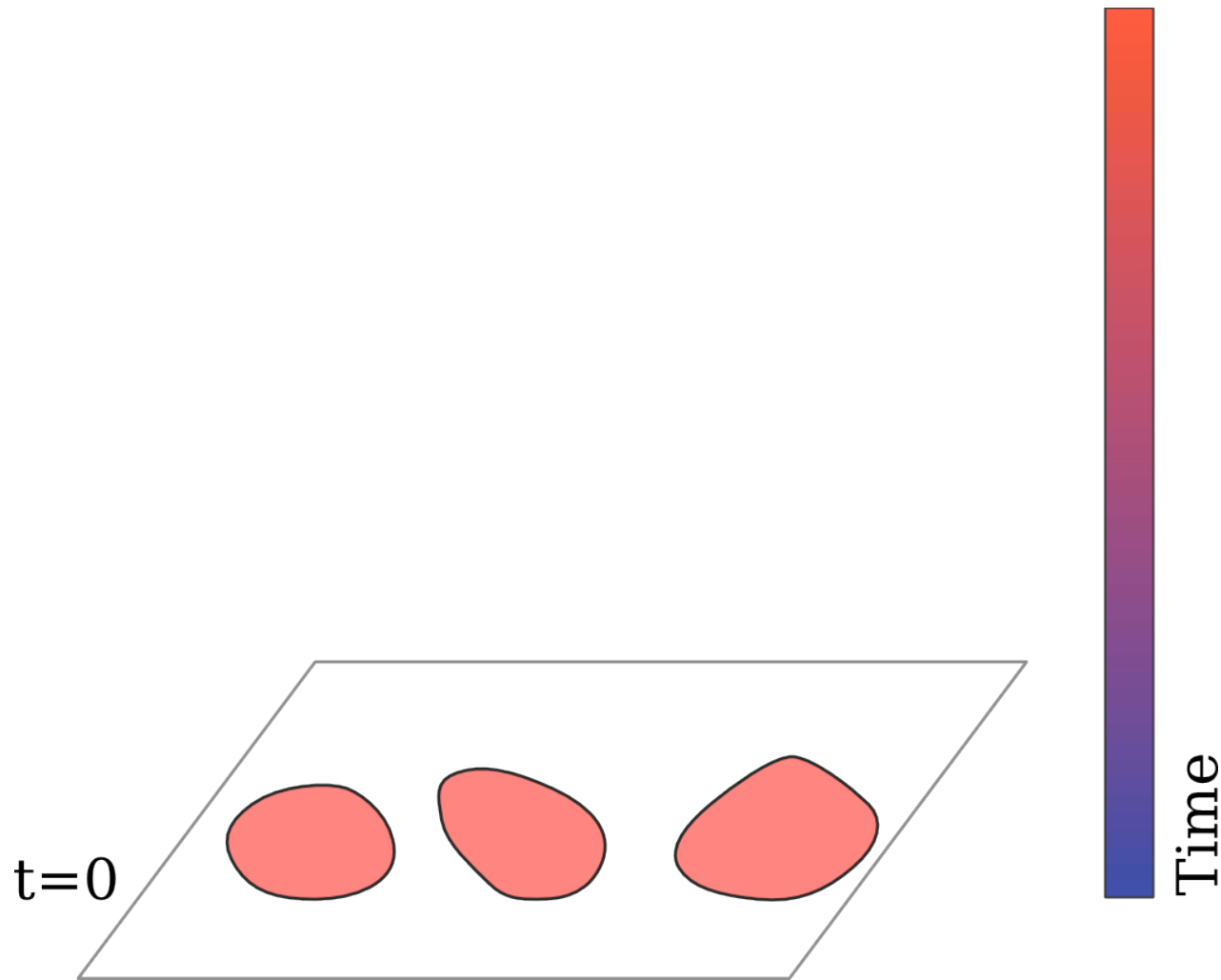


domain

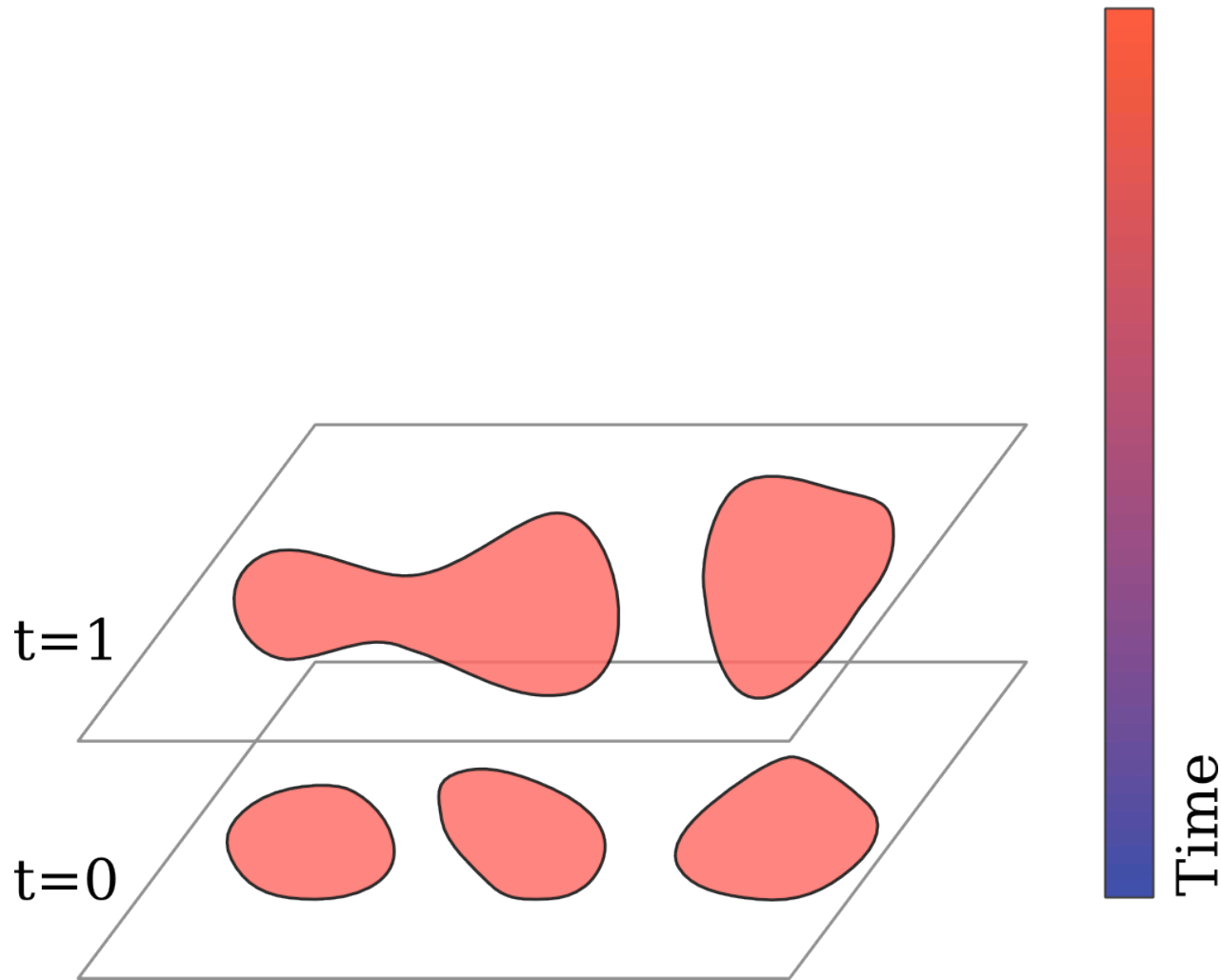


hierarchy

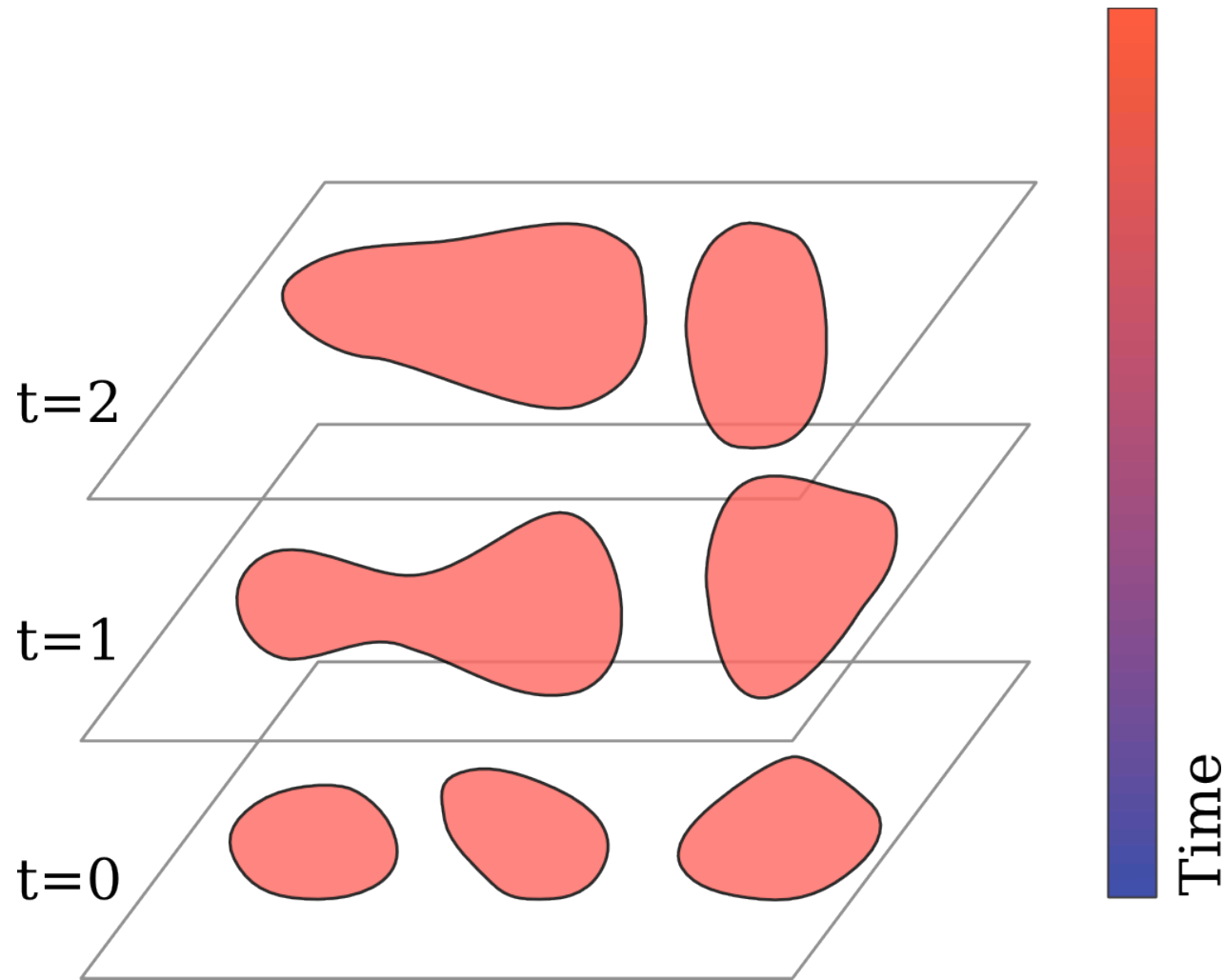
We track in time by interpolation in 4D and contraction to a graph (Reeb Graph)



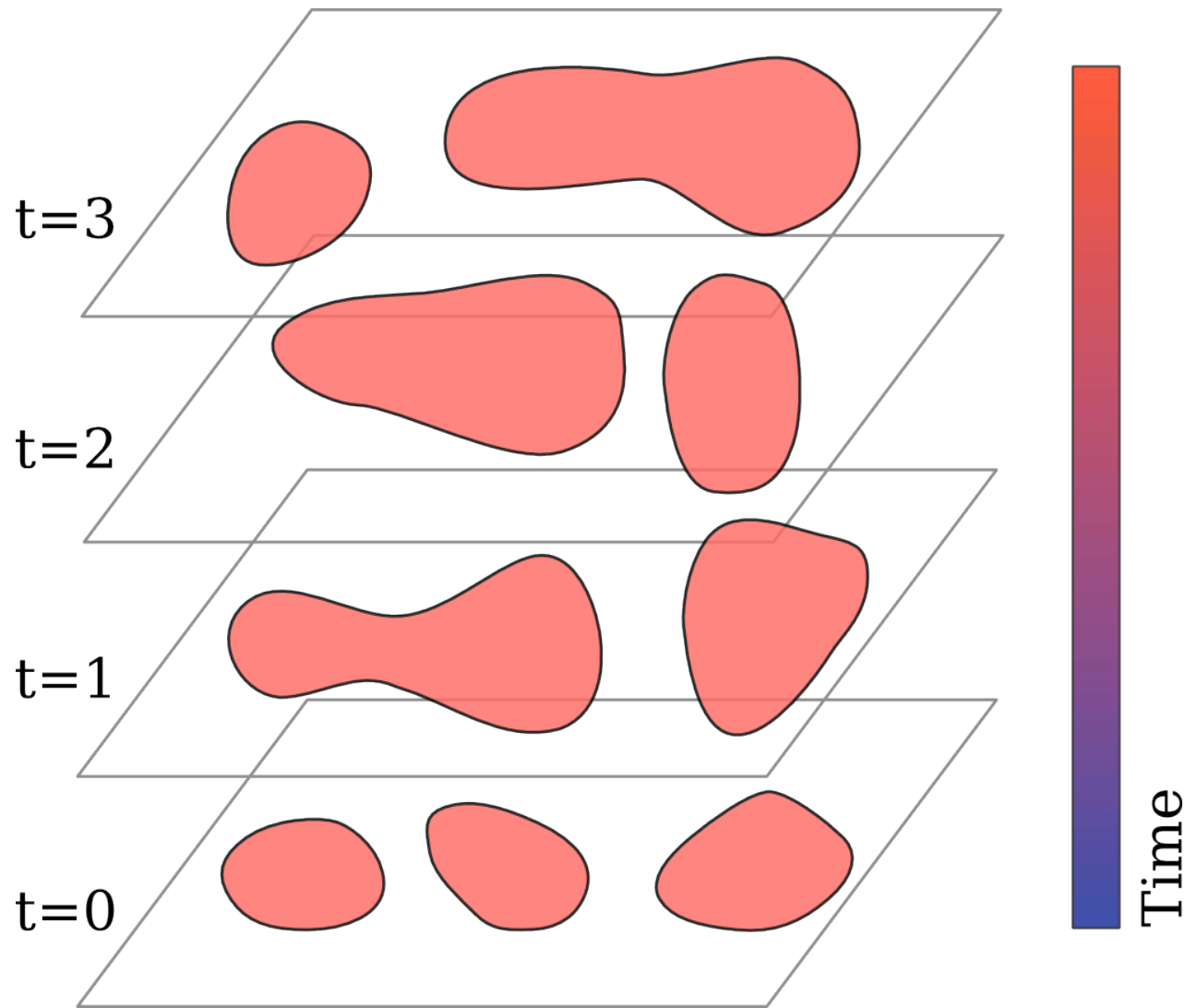
We track in time by interpolation in 4D and contraction to a graph (Reeb Graph)



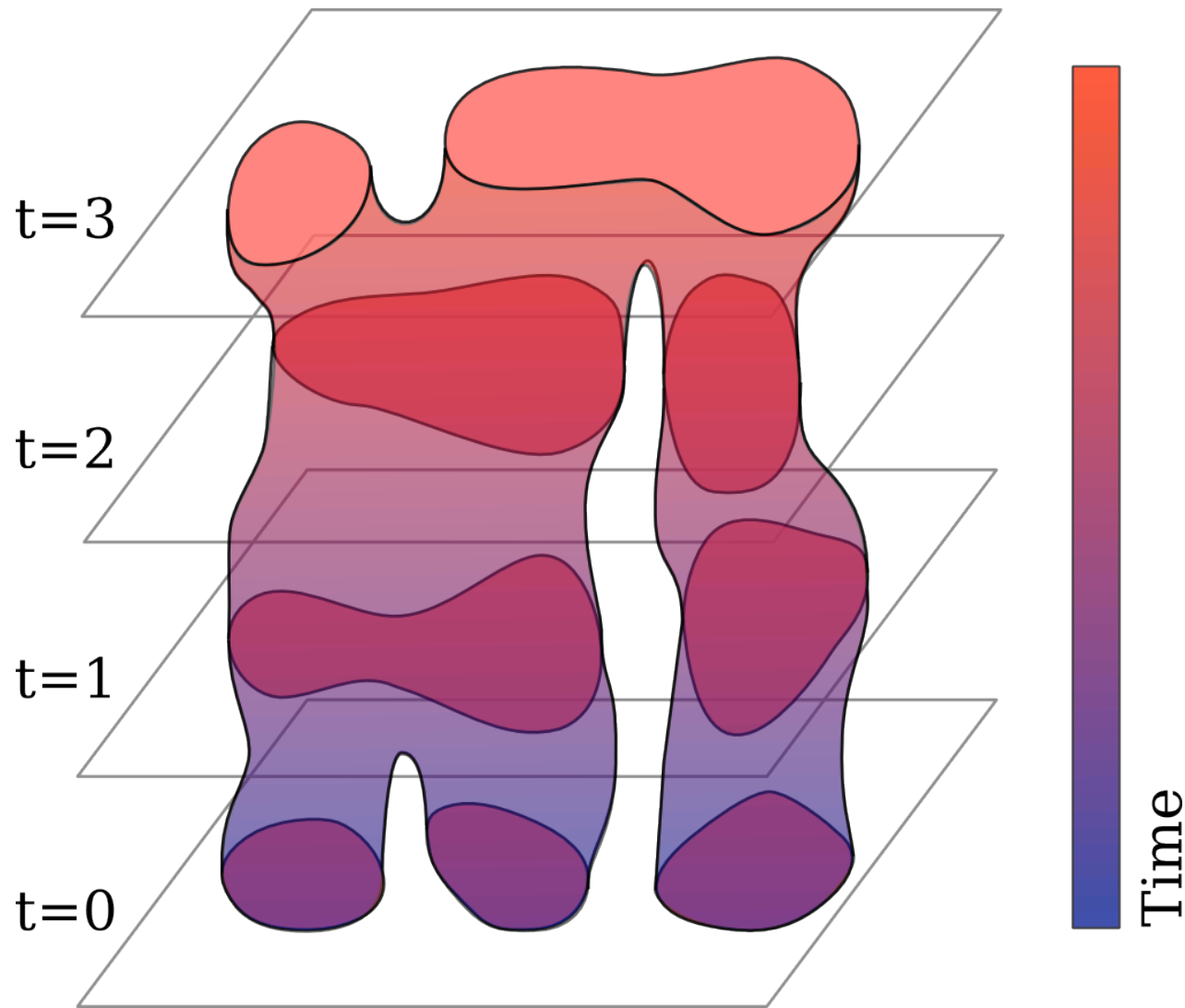
We track in time by interpolation in 4D and contraction to a graph (Reeb Graph)



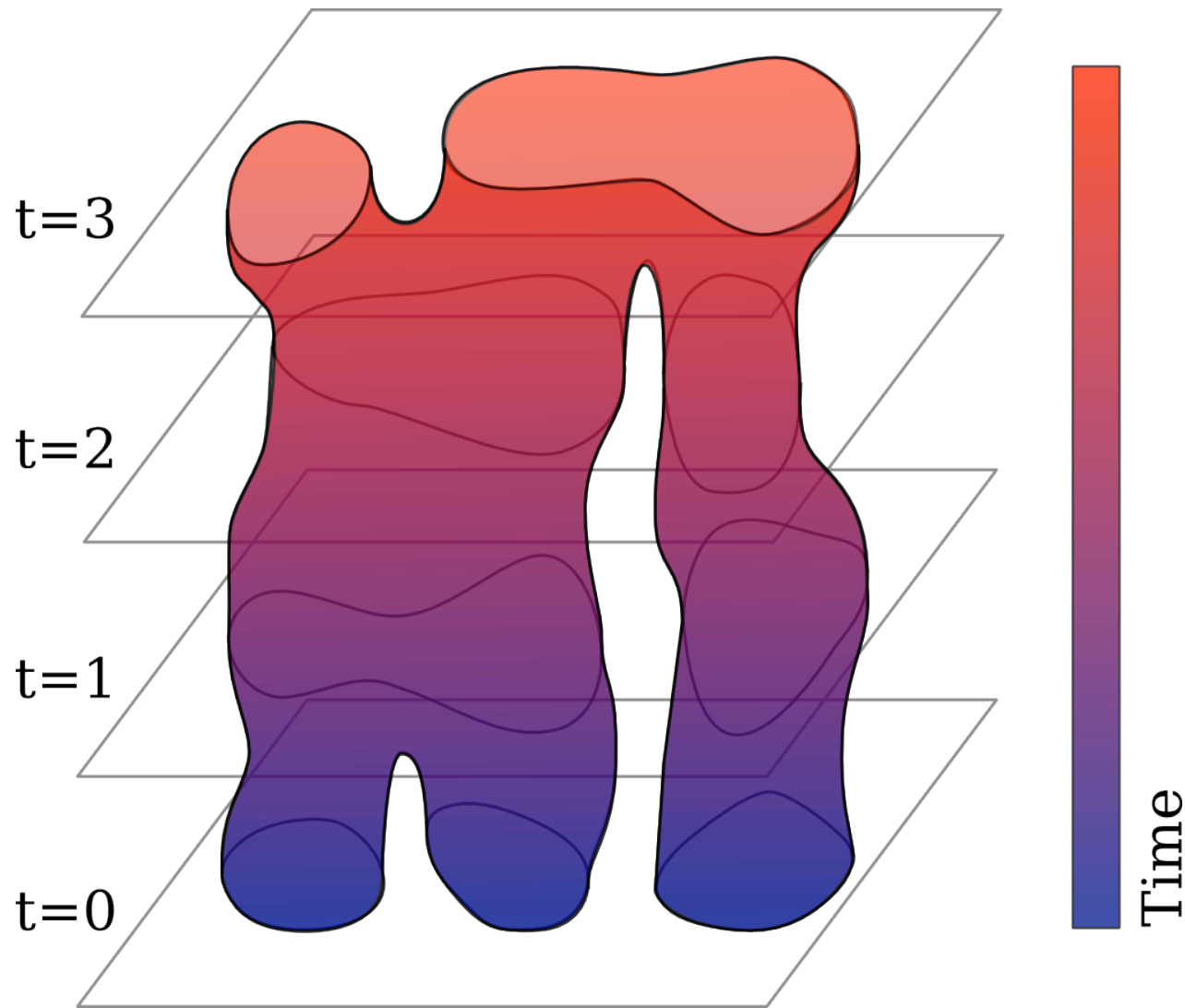
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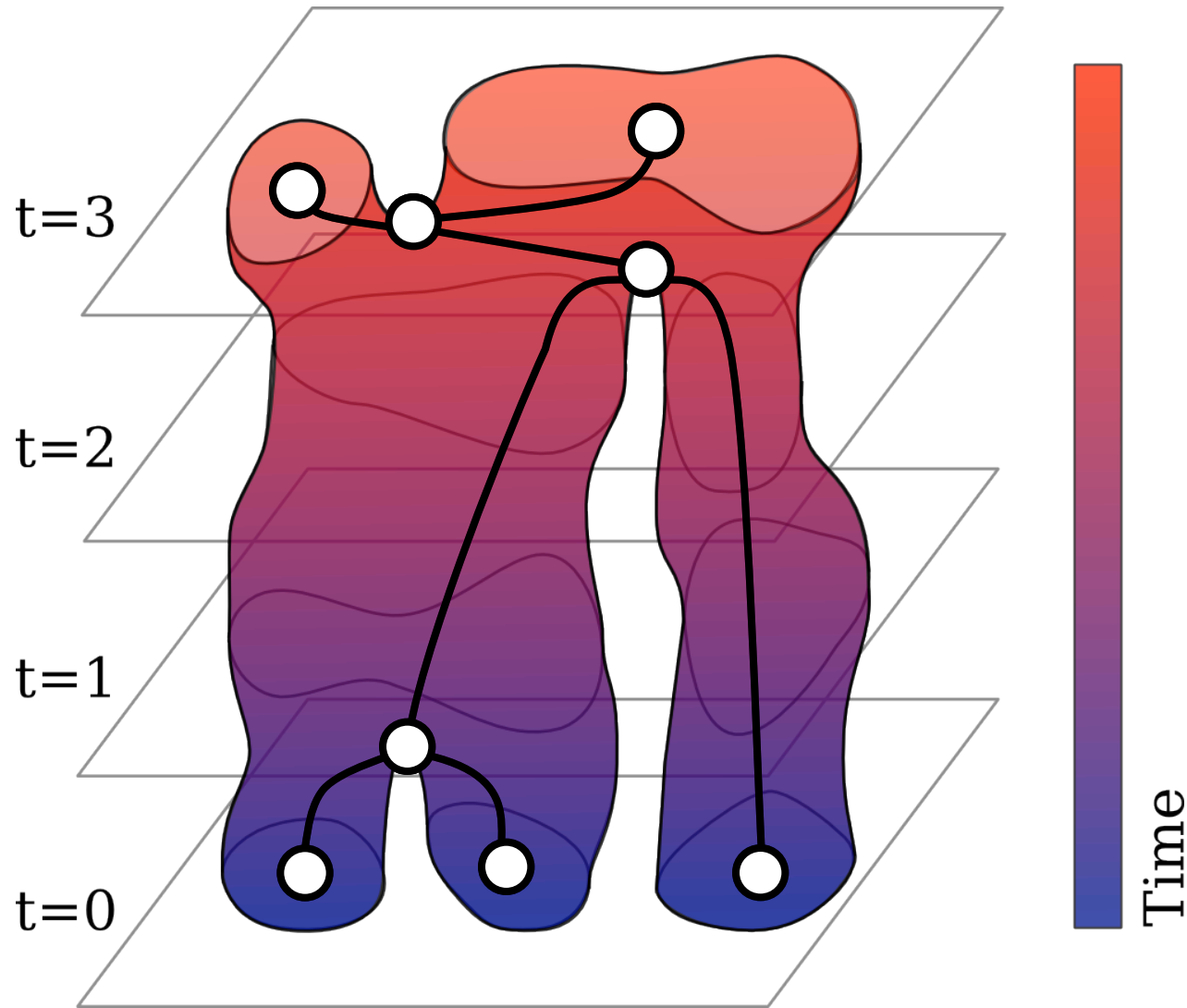
We track in time by interpolation in 4D and contraction to a graph (Reeb Graph)



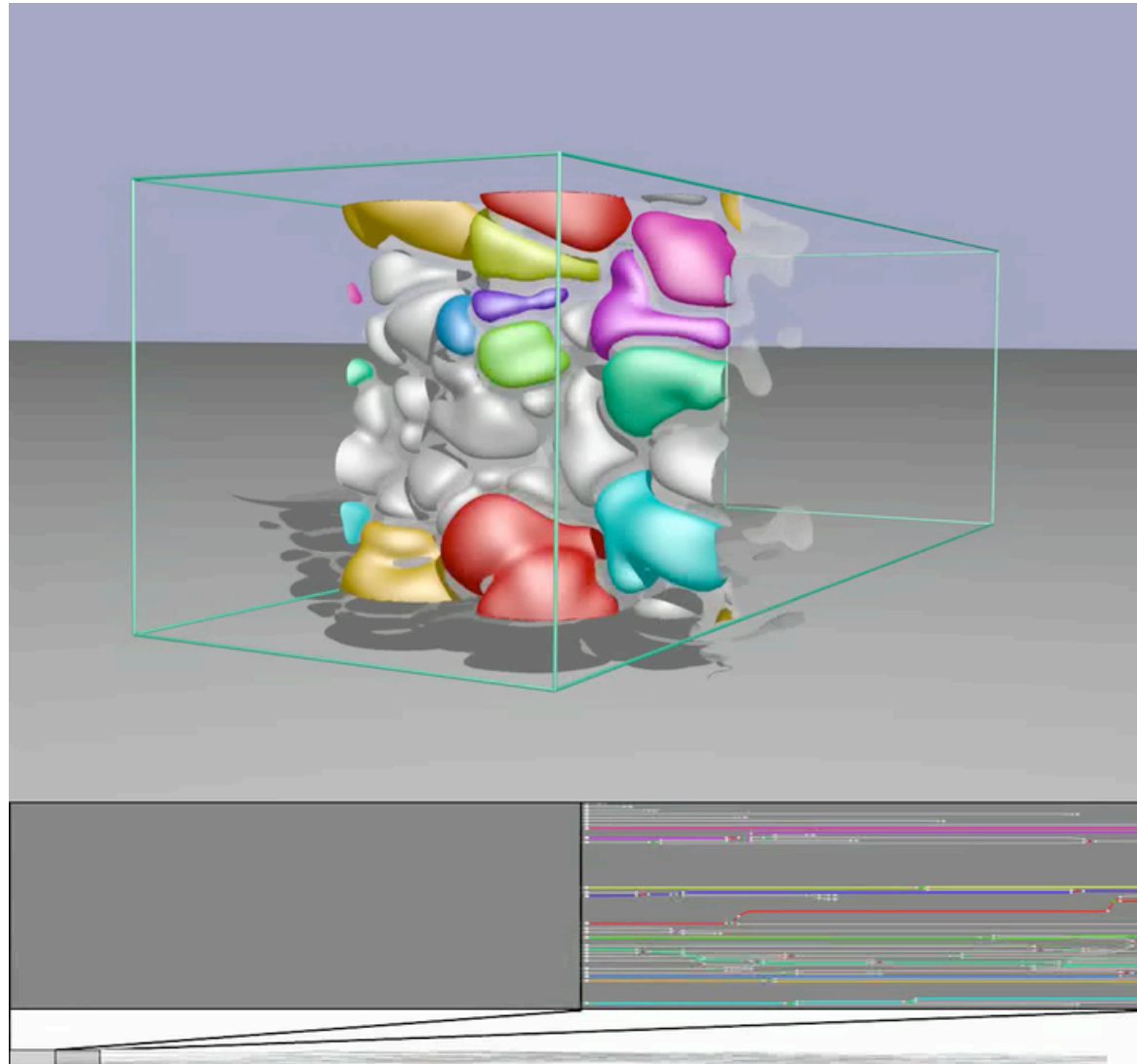
We track in time by interpolation in 4D and contraction to a graph (Reeb Graph)



We track in time by interpolation in 4D and contraction to a graph (Reeb Graph)



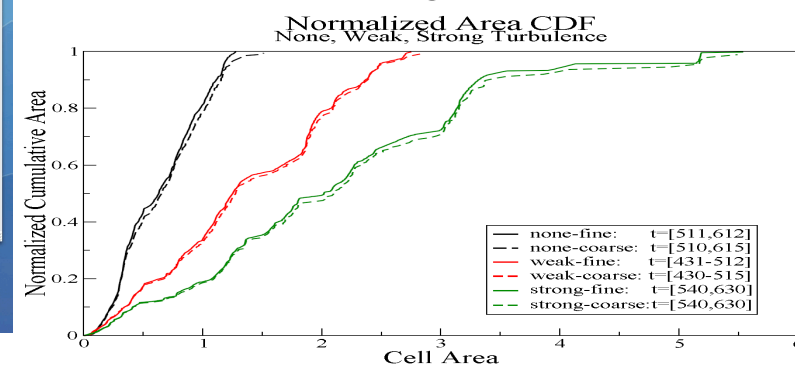
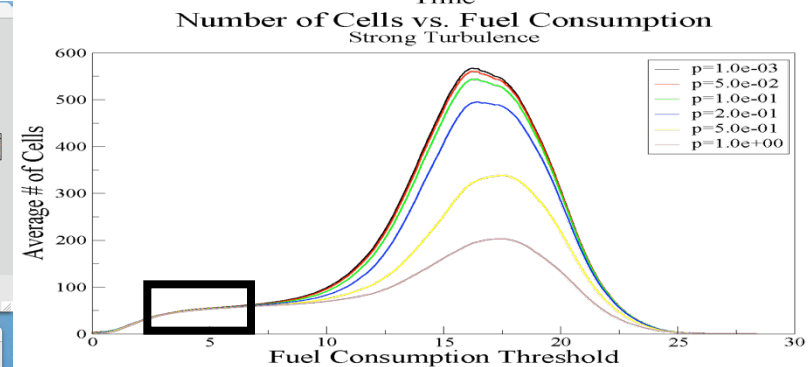
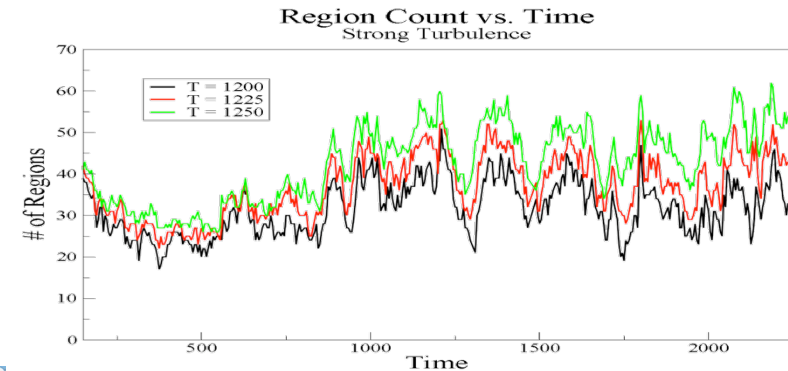
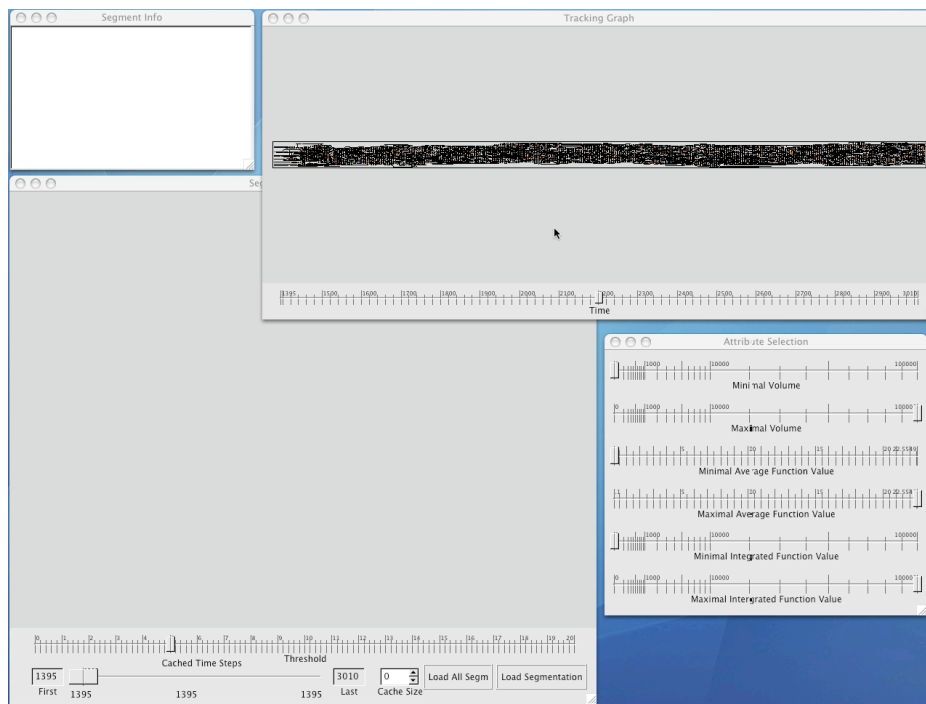
Each Set of Parameters Results in a Robust Segmentation and Tracking of Burning Cells



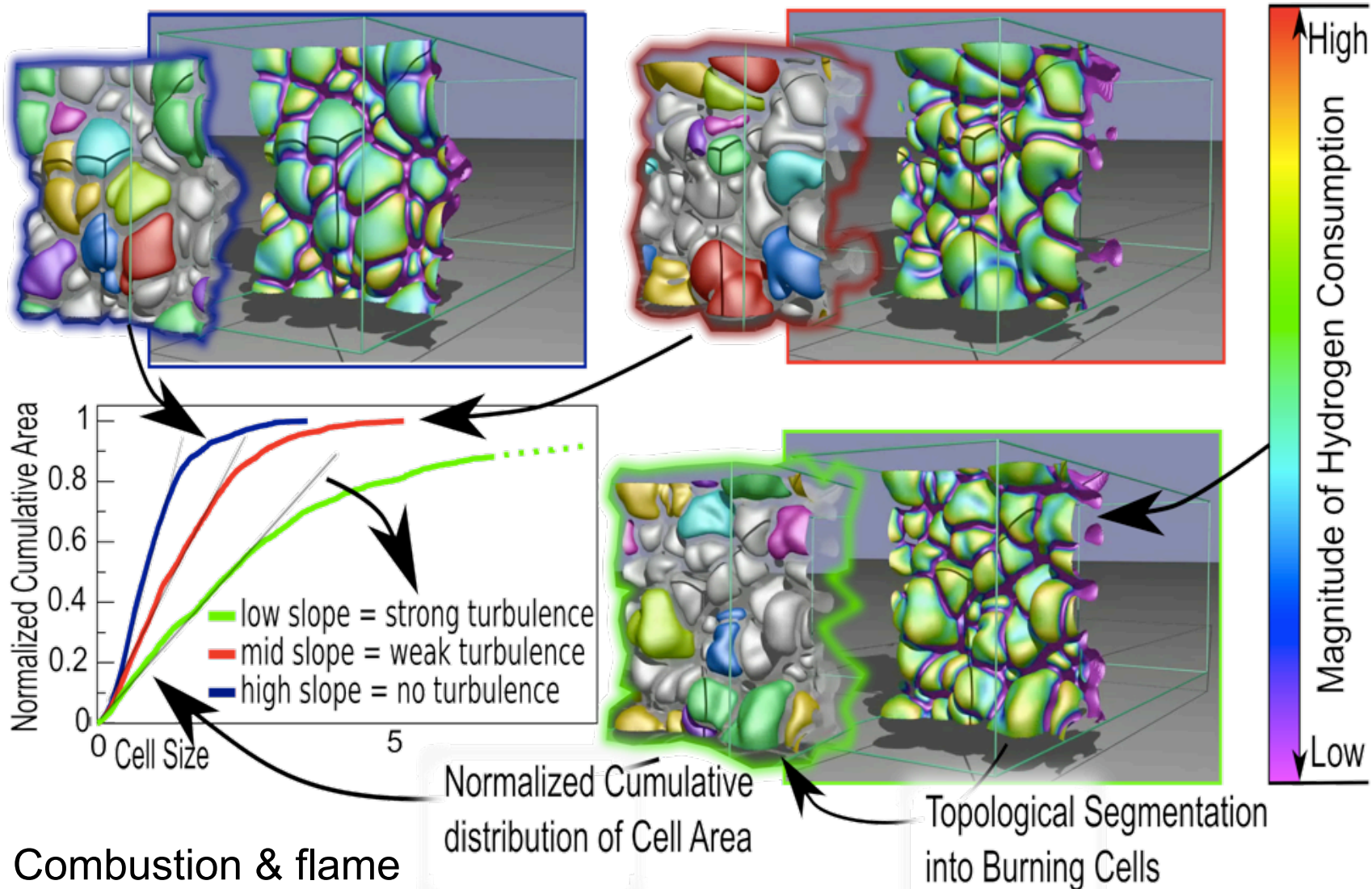
We Allow Exploration of the Full Space of Parameters Defining the Features



- interactive exploration
- comparison of statistics



Topological Segmentation Allows to Quantify Turbulence as Slope of the Area Distributions



- Combustion & flame

VACET Enabled Virtuous Cycle of Science Driven Technology Creation and Deployent



- **Tight connection between:**
 - basic (science driven) research
 - software deployment
 - user support
- **Joint publications:**
 - science and vis publications
- **Focused technical approach:**
 - performance tools for fast data access
 - general purpose data exploration
 - error bounded quantitative analysis
 - feature extraction and tracking
- **The path forward:**
 - topological co-processing embedded in simulations to save compact information with more expressive power
 - unified representation of features in the space-time continuum
 - feature based comparison of simulations experiments
 - extensions to steady and unsteady vector fields

